

2-Hydroxy-3,5-dimethylcyclopent-2-en-1-one

Other names:	2-Cyclopenten-1-one, 2-hydroxy-3,5-dimethyl- 2-Hydroxy-3,5-dimethyl-2-cyclopenten-1-one
Inchi:	InChI=1S/C7H10O2/c1-4-3-5(2)7(9)6(4)8/h4,9H,3H2,1-2H3
InchiKey:	RLEJFFGSMZQXJX-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	CC1=C(O)C(=O)C(C)C1
Mol. weight [g/mol]:	126.15
CAS:	21834-98-0

Physical Properties

Property code	Value	Unit	Source
gf	-204.10	kJ/mol	Joback Method
hf	-382.42	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.427		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1093.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1702.00		NIST Webbook
tb	543.96	K	Joback Method
tc	749.04	K	Joback Method
tf	334.39	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.68	J/molxK	543.96	Joback Method
cpg	249.51	J/molxK	578.14	Joback Method

cpg	259.90	J/mol×K	612.32	Joback Method
cpg	269.85	J/mol×K	646.50	Joback Method
cpg	279.33	J/mol×K	680.68	Joback Method
cpg	288.35	J/mol×K	714.86	Joback Method
cpg	296.89	J/mol×K	749.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21834980&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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